6,7-Dehydrohyoscyamine

Inchi: InChI=1S/C17H21NO3/c1-18-13-7-8-14(18)10-15(9-13)21-17(20)16(11-19)12-5-3-2-4-6-
InchiKey: NZJZSPMNEYIORP-UHFFFAOYSA-N
Formula: C17H21NO3
SMILES: CN1C2C=CC1CC(OC(=O)C(CO)c1ccccc1)C2
Mol. weight [g/mol]: 287.35
CAS: 61616-97-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Crippen Method
logp	1.707		Crippen Method
mcvol	223.900	ml/mol	McGowan Method
rinpol	2201.10		NIST Webbook
rinpol	2201.10		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C61616975&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices